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The effect of nitrogen and argon dilution on methane oxidation in laminar flames

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Abstract

Numerical simulation of dilution effect on combustion and flame properties is desirable for various industrial or scientific applications. Predicative capabilities of the simplified (one- and two-step) chemical kinetic mechanisms of methane oxidation in highly diluted flames were evaluated on the basis of mathematical modelling in one-dimensional (axisymmetric) configuration. Profiles of temperatures and concentrations of reactants, combustion products and intermediates in premixed flat flame and nonpremixed counterflow flame burning methane and air/diluent mixture were determined. Detailed chemical kinetic modelling was performed additionally in order estimate the flame temperature and speciation and to quantify the effect of elevated argon and nitrogen concentration and oxygen deficiency on diluted combustion. Global chemical kinetic models were implemented into computational fluid dynamics tool to approve their applicability for numerical simulations of diluted flames in more complex geometries.

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Keywords: Dilution; methane oxidation; global chemistry; model; laminar flame

1. Introduction

Dilution with nitrogen or argon is a simple way of influencing the parameters of combustion and decreasing the temperature of flame, which may be desirable for some industrial (e.g. pharmaceutical) or scientific applications (e.g. in analytical chemistry [1]). Safety aspects of dilution phenomena are of pronounced importance in the context of: (i) inertization of process units in order to avoid the ignition or self-ignition; (ii) early suppression of explosion phenomena; (iii) extinguishment of fires in enclosures. Dilution is also used for eliminating the soot formation in combustion chemistry related laboratory experiments, when soot-free flame conditions are favourable for optical or probe diagnostics and modelling complexity needs to be eliminated.

Dilution reduces the rates of chemical reactions by introducing additional inert mass of argon atoms or nitrogen molecules. Decreased concentration of reactants limits the number (probability) of effective collisions. Furthermore, heat capacity relevant to diluent gas affects local thermophysical properties in flame implying further changes in chemical kinetics. The effect of dilution on the structure of reaction zone differs with respect to the geometry and boundary conditions appropriate for the given combustion system. According to the concept of experimental and computational investigations, commonly adopted in the field of combustion related research [2,3], two basic configurations of laminar flame (see Fig. 1.) will be considered in the following text:

- premixed flat-flame
- nonpremixed counterflow (opposed-jet) flame

This work is aimed at development of approaches suitable for modelling the coupled phenomena of chemical kinetics and fluid flow physics in the environment of flames at specific combustion conditions. Implementation of simplified chemical kinetics into the computational fluid dynamics (CFD) tools is relatively efficient way, which enables to predict the parameters of combustion even in highly complex geometry and specific conditions of laboratory or industrial burners [4-9]. However, testing the performance of selected global chemistry model against the detailed kinetic mechanisms in the simplified geometry of zero-dimensional reactor or one-dimensional flame is the most important step of validation procedure. To recent author's knowledge, any comparative study of global chemistry models was performed for diluted laminar flames.

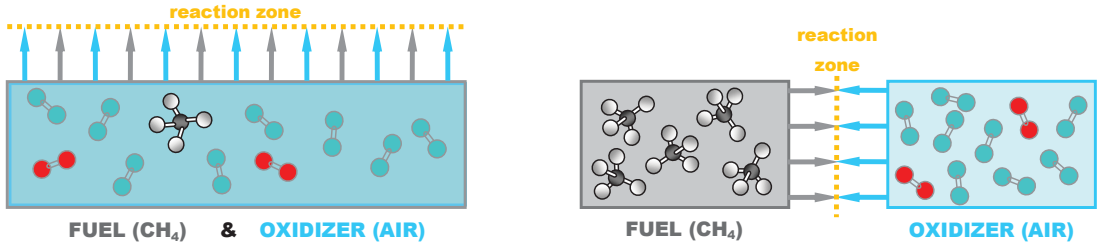

Fig. 1. Illustrative structure of (a) stoichiometric premixed methane – air flat flame; (b) nonpremixed methane/air counterflow flame.

Nomenclature

A	pre-exponential factor
a	stain rate
E_a	activation energy
k	rate constant of chemical reaction
p	atmospheric pressure
R	universal gas constant
T	absolute temperature
s_L	laminar flame speed
v_f	velocity at fuel inlet
v_{fox}	inlet velocity of fuel-air-diluent mixture at burner exit
v_{ox}	velocity at oxidizer inlet
$X(Ar)$	volume fraction of argon in air
$X(Ar)_{ext}$	minimum extinguishing volume fraction of argon in air
$X(CH_4)$	volume fraction of methane
$X(N_2)_{ext}$	minimum extinguishing volume fraction of nitrogen in air
$X(O_2)$	volume fraction of oxygen
z	computational axis coordinate
β	temperature exponent

2. Methodology

The main purpose of this study is to test the performance of global (one-step and two-step) chemical kinetics models available in literature for the specific conditions of argon and nitrogen diluted flame. Steady-state structure of laminar nonpremixed counterflow (opposed-jet) flame and premixed flat flame was predicted. Moreover, laminar flame speeds (burning velocities) in premixed flame were estimated for each chemical kinetic model and conditions selected. One-dimensional simulations were performed using Cantera 1.7 (an object-oriented open-source software toolkit for chemical kinetics, thermodynamics, and transport processes [10]).

Finally, selected global chemical kinetic model was implemented into the ANSYS Fluent 14.0 (commercial multi-purpose tool for simulations of computational fluid dynamics). As a representative case study, laminar nonpremixed counterflow flame moderately diluted by argon was simulated at conditions comparable to one-dimensional configuration.

The detailed description of these mathematical modelling tools is out of the scope of this contribution. Only briefly, we can summarize that both software tools enable to numerically solve the set of ordinary differential equations describing balance of vector and scalar variables in the chemically reacting flows. Governing equations for conservation of mass, energy, species and momentum are solved in cylindrical (z-axis) coordinates in the case of calculations using Cantera 1.7 and in planar (x- and y-axis) coordinates

in the case of CFD simulations performed in ANSYS Fluent 14.0. The parameters of chemical kinetics, thermodynamic and transport properties employed in the frame of this study are presented in the following text as well as boundary conditions applied for the simulations.

Parameters of single irreversible methane oxidation reaction provided by Puri and Seshadri [11] (with pre-exponential factor modified by Renner [12]) and the set of constants optimized for nonpremixed combustion by Zambon and Chelliah [13] were used as representative one-step models.

Two-step oxidation mechanisms include reversible reaction of carbon monoxide with oxygen after the initial fuel oxidation step. Based on bibliographic research, rate constants and reaction orders proposed by Westbrook and Dryer [14] (including the rate constants reported in [15]) and Bibrzycki and Poinsot [16] were selected for this study. The abbreviations were assigned to the models according to first letters of authors or the name stated in the adequate publications. All the kinetic parameters are reported in "cgs" unit system, which is broadly preferred in the community of combustion scientists and engineers. The conversion of pre-exponential factor to "SI" unit system (if necessary) should be handled carefully considering properly the reaction order.

In the case of global kinetic mechanisms, the constants of Arrhenius equation, see Equation (1), are often supplemented by the modified reaction-order constants different from the stoichiometric coefficients for any of species present in the mechanism, see Table 3 and Table 4.

$$k = A\, T^{\beta} \exp(-E_a/RT) \tag{1}$$

Table 1. One-step ZC model of methane oxidation (units in cm, s, cal, and mol)

Reaction and stoichiometry	A	β	E_a	Reaction orders	Reference
$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O$	1.35×10^{20}	0	3.00×10^{4}	$[CH_4][O_2]^2$	[13]

Table 2. One-step PS model of methane oxidation (units in cm, s, cal, and mol)

Reaction and stoichiometry	A	β	E_a	Reaction orders	Reference
$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O$	3.00×10^{22}	0	4.50×10^{4}	$[CH_4][O_2]^2$	[12]

Table 3. Two-step WD model of methane oxidation (units in cm, s, cal, and mol)

Reaction and stoichiometry	A	β	E_a	Reaction orders	Reference
$CH_4 + 1.5\ O_2 \rightarrow CO + 2\ H_2O$	1.59×10^{13}	0	4.78×10^{4}	$[CH_4]^{0.7}[O_2]^{0.8}$	[15]
$CO + 0.5\ O_2 \rightarrow CO_2$	3.98×10^{14}	0	4.07×10^{4}	$[CO][O_2]^{0.25}[H_2O]^{0.5}$	[15]
$CO_2 \rightarrow CO + 0.5\ O_2$	5.00×10^{8}	0	4.07×10^{4}	$[CO_2]$	[14]

Table 4. Two-step CM model of methane oxidation (units in cm, s, cal, and mol)

Reaction and stoichiometry	A	β	E_a	Reaction orders	Reference
$CH_4 + 1.5\ O_2 \rightarrow CO + 2\ H_2O$	2.00×10^{15}	0	3.50×10^{4}	$[CH_4]^{0.9}[O_2]^{1.1}$	[16]
$CO + 0.5\ O_2 \rightarrow CO_2$	2.00×10^{9}	0	1.20×10^{4}	$[CO][O_2]^{0.5}$	[16]
$CO_2 \rightarrow CO + 0.5\ O_2$	8.11×10^{10}	0	7.72×10^{4}	$[CO_2]$	[16]

Reaction orders are allowed to have non-integer value, but need to be positive in order to enable the solution in the default algorithm available in Cantera (treatment of numerical problems relevant to possibility of zero value in denominator of reaction rate is not implemented in current version of the code). Moreover, if reaction orders of reversible reactions are not equal to stoichiometric coefficients, rate constants of reverse reaction should be explicitly defined as an input parameter for simulation in Cantera.

Detailed mechanism of methane oxidation (GRI-Mech 3.0 [17]) was utilized for numerical simulations in Cantera toolbox. This chemical kinetic mechanism (abbreviated further GRI30) is broadly validated in the range of conditions employed here. Therefore it can serve as the realistic estimate of temperature and concentration profiles having the reliability comparable to experimental data. Thermodynamic constants and transport data of the individual species used in our simulations were those compatible with GRI30 mechanism. The set of chemical kinetics, thermodynamic and transport properties described above were implemented into the Cantera software toolbox through creation of *.cti (Cantera input) files by converting the relevant data initially prepared in so-called Chemkin format.

Multicomponent diffusion model (the set of binary diffusion coefficients expressed from kinetic theory used to describe the transport properties of species) was employed for estimating temperature dependent transport properties of individual species. The results of simulation employing simplified mixture-averaged transport model (averaged diffusion coefficients for each component used to describe the transport properties of gaseous species) are reported for burner-stabilized premixed flat flame. Cantera simulations of highly diluted premixed flat flame using multicomponent transport model did not lead to the successive solution (iteration process was aborted after prolonged simulation time). Nevertheless, only minor difference in prediction between multicomponent and mixture-based transport model are expected regarding the results of laminar burning velocity calculation. Gravitational force was not taken into account as well as heat radiation, which was neglected through all the simulations performed. Only atmospheric pressure flames were considered in this study.

3. Results and discussion

Profiles of temperatures and concentrations of reactants, combustion products and intermediates in nonpremixed counterflow flame and premixed flat flame configurations were determined based on mathematical modelling.

Computational domain of 20 millimetres length was utilized and uniform grid consisting of 201 points separated by 0.1 mm was retained during the entire iteration process (grid refinement functionality disabled) in Cantera. The positions of inlets at computational coordinate are $z = 0$ for fuel stream and $z = 0.02$ m for oxidized stream. Fixed value of mass flow rate specified at gas inlets as boundary condition. Equal exit velocities of opposed fuel and oxidizer jets ($v_f = -v_{ox} = 0.25$ m/s) were used for the nonpremixed counterflow flame simulations.

The burner-stabilized stoichiometric methane-air premixed flat flame were simulated at burner exit velocities $v_{fox} = 0.125$ cm/s. The selection of the given conditions can be reasoned by the low laminar flame speed at high argon and nitrogen dilution, which is of comparable magnitude to flow velocity. In this case the inlet of fuel-oxidizer mixture is placed at $z = 0$ point.

The temperature of 300 K and the atmospheric pressure ($p = 101325$ Pa) are set as the initial conditions at gas inlets for all the simulations performed in Cantera. The composition of gaseous species utilized for each of simulated case is specified in the Table 5 and Table 6. One-dimensional simulation of highly diluted flames were performed at initial conditions corresponding to 90% of minimum extinguishing volume fractions of argon and nitrogen in air being $X(Ar)_{ext} = 0.373$ and $X(N_2)_{ext} = 0.259$ respectively, as determined by Takahashi et al. [18] employing cup-burner apparatus.

Table 5. Composition of fuel and oxidizer (-diluent) mixture used for nonpremixed flame simulations

Simulation case (Fuel/Oxidizer-Diluent)	Mole fraction at fuel inlet (-)	Mole fractions at oxidizer inlet (-)
CH_4/Air	$X(CH_4) = 1$	$X(O_2) = 0.21$; $X(N_2) = 0.79$
CH_4/Air-Ar	$X(CH_4) = 1$	$X(O_2) = 0.139$; $X(N_2) = 0.525$; $X(Ar) = 0.336$
CH_4/Air-N_2	$X(CH_4) = 1$	$X(O_2) = 0.161$; $X(N_2) = 0.839$

Table 6. Composition of fuel-oxidizer (-diluent) mixture used for premixed flame simulations

Simulation case (Fuel-Oxidizer-Diluent)	Mole fractions at burner inlet (-)
CH_4-Air	$X(CH_4) = 0.0950$; $X(O_2) = 0.190$; $X(N_2) = 0.715$
CH_4-Air-Ar	$X(CH_4) = 0.0650$; $X(O_2) = 0.130$; $X(N_2) = 0.490$; $X(Ar) = 0.315$
CH_4-Air-N_2	$X(CH_4) = 0.0745$; $X(O_2) = 0.149$; $X(N_2) = 0.7765$

3.1. Simulations of undiluted (CH_4/Air) flames

One-dimensional flame simulations using Cantera toolbox were focused in the first step on the prediction of the structure of reaction zone not affected by the dilution. Temperature profiles in nonpremixed flame are overestimated significantly for all global chemistry models, see Fig. 2.(a). On the fuel lean side of reaction zone, all the models predict the temperature in agreement with detailed GRI30 model. The shifted position of temperature maxima towards the oxidizer inlet is less pronounced for the one-step models. This is an opposite for the temperature profiles in premixed flames where one-step models give poor prediction, see Fig. 2.(b). Mainly ZC model (having slightly lower pre-exponential factor and lower activation energy then PS model) shows rather slow reaction rate. However, it should be noted that the Arrhenius constants for this model was optimized for nonpremixed flame [13], where this setup lead to reduced overestimation of maximum temperature in the reaction zone.

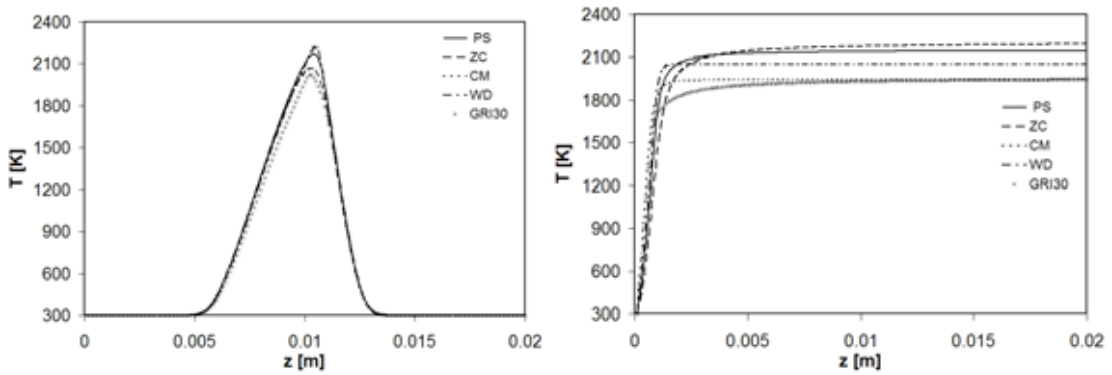

Fig. 2. Predicted profiles of temperatures in (a) CH_4/Air nonpremixed counterflow flame; (b) CH_4-Air premixed flat flame

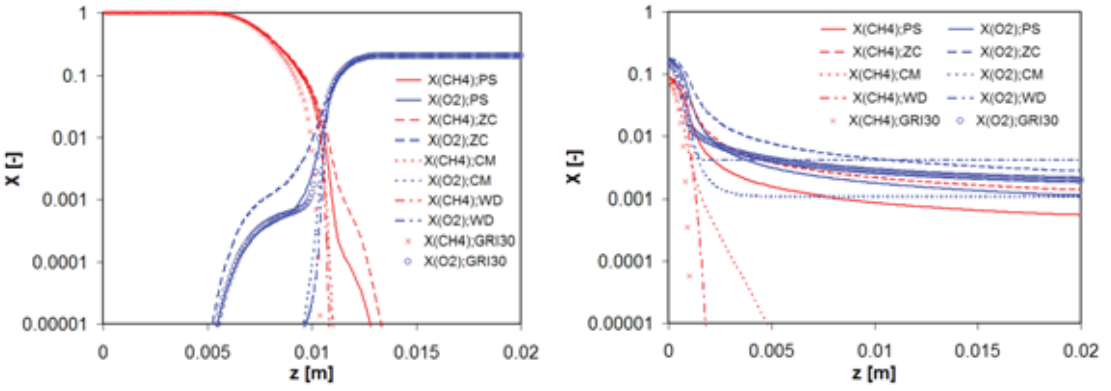

Fig. 3. Predicted volme fraction profiles of reactants in (a) CH_4/Air nonpremixed counterflow flame; (b) CH_4-Air premixed flat flame

Temperature in post-combustion region of premixed flame is precisely predicted by two-step CM model. The deviation from detailed kinetic mechanism in temperature rise region (reaction zone) is expected at this level of simplification. The plots of volume fractions of the reactants, $X(CH_4)$ and $X(O_2)$ shown in logarithmic coordinates, indicate slow fuel consumption compared to detailed kinetics for all the global models, see Fig 3.(a). So called "fuel-leakage" effect, which is the artefact linked to the global one-step models, lead to inflection of concentration curve on the fuel-lean side of the reaction zone. On the other side, penetration of oxygen to fuel-rich region of the nonpremixed flame, called "oxygen-leakage" effect is expected to occur as predicted by detailed kinetic model. This effect if of critical importance at reduced temperature conditions, as will be discussed below for diluted flames.

The concentration of reaction intermediate (only CO considered) and products (CO_2 and H_2O) in nonpremixed flame is reasonably predicted by two-step models, which is mainly the case of H_2O concentration, see Fig. 4.(a). The peak CO_2 concentration in the reaction zone is overestimated by WD model by similar magnitude as CO concentration is underestimated.

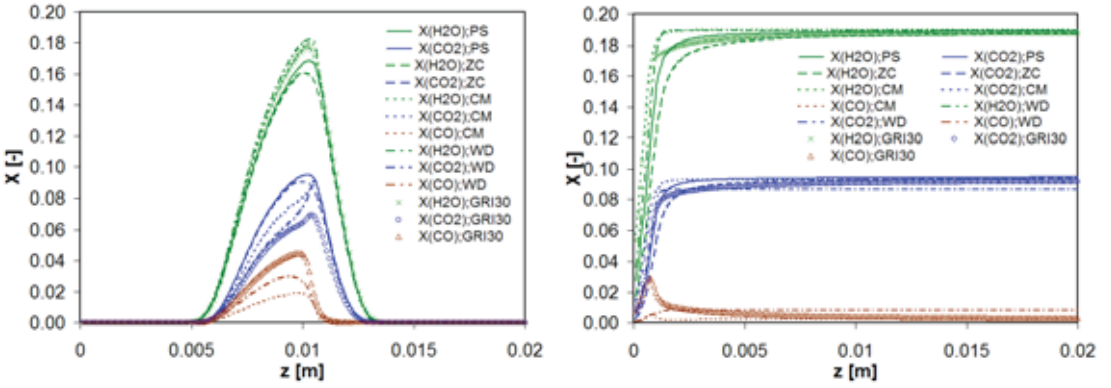

Fig. 4. Predicted volume fraction profiles of products and intermediate in (a) CH_4/Air nonpremixed counterflow flame; (b) CH_4-Air premixed flat flame

Analogous, but inverse deviation of CO/CO_2 concentration ratio were observed in the results of premixed flame simulation, see Fig. 4.(b). These findings support the hypothesis, that the equilibrium constant (the ratio of forward and reverse reaction rate) for reversible CO oxidation is improperly adjusted for high temperature region in this mechanism. Similar deviations of CO and CO_2 concentration profiles in nonpremixed flame are obtained from the second two-step (CM) model. Nevertheless, the prediction of speciation in post-combustion region of premixed flame given by CM model agrees well with the data obtained using detailed chemistry model.

3.2. Simulations of highly diluted (CH_4/Air-Ar) flames

Temperature profiles in argon diluted nonpremixed flames given by one-step models show serious underestimation leading to temperatures near to 1550 K, which is reported to be the limit for sustaining the combustion in this configuration [19]. Decreased concentration of oxygen in oxidizer stream together with argon heat extraction leads to unrealistic estimation of fuel consumption rate in peak temperature region and distortion of parameters of reaction zone in highly diluted nonpremixed flame. Predictions given by one-step models can be mainly characterized by increased fuel leakage and shift of the temperature and species concentration gradient region on fuel-lean side (as well as the position of given maxima) towards the fuel inlet, see Fig. 5.(a).

The performance of two-step models in nonpremixed flame is not changed drastically compared to flames without dilution. All the quantities predicted by two-step models for nonpremixed flame are qualitatively comparable to the case without dilution regarding the deviations of results from the GRI30 model. For the premixed flame, only the results of simulation using CM model together with the results of GRI30 are reported, as the application of other global chemistry models was unsuccessful in that case (iteration process did not lead to the successive solution and was aborted after prolonged time period). This fact can be rationalized by the slow laminar burning velocities ($s_L < v_{fox}$) provided under the high dilution conditions by these models (ZC, PS, WD), see Table 7 in Section 3.4.

In the case of non-premixed flame the dilution effect resulting in temperature reduction and decreasing combustion rate enables molecular oxygen to penetrate through the peak flame temperature region to the fuel side of reaction zone. The effect of partial pre-mixing caused by “oxygen leakage” is known to change the structure of nonpremixed flame. The profiles of intermediate species as well as sooting behavior of flame are affected seriously by this phenomenon [20,21]. The ability of global chemistry models to capture oxygen leakage in argon diluted flame is the important measure of their applicability for the computational studies focused on this point. We can summarize briefly, that the increase of oxygen concentration on fuel-rich side compared to the flame without dilution is captured by one-step models in reasonable accordance to detailed chemistry model. On the other hand, two-step models used in our study and mostly the CM model crudely underpredicts the effect of oxygen leakage.

3.3. Simulations of highly diluted (CH_4/Air-N_2) flames

The performance of global models in nitrogen diluted flames is qualitatively similar to previous (argon diluted) case. Considerable lack of predicative capabilities of one-step models in premixed flames is in analogy. The agreement of CM model prediction with the detailed chemistry model is even better in the case of nitrogen dilution. Nevertheless, the underprediction of temperature profile and overprediction of fuel leakage is not so serious in the given case. Reasonable prediction of the important parameters describing the reaction zone of nitrogen diluted nonpremixed flame (mainly the temperature and oxygen concentration) are obtained using one-step PS model.

The results of simulation for all highly diluted flames are summarized here below (Fig. 5. – Fig 10.).

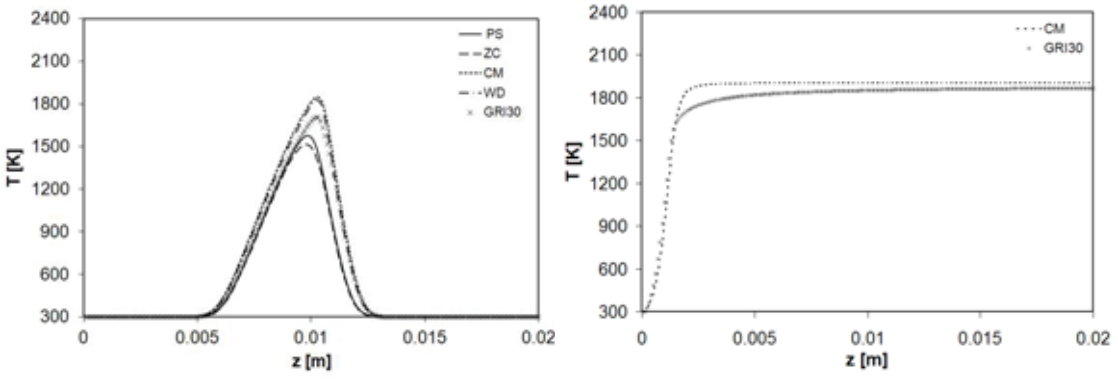

Fig. 5. Predicted profiles of temperatures in (a) CH_4/Air-Ar nonpremixed counterflow flame; (b) CH_4-Air-Ar premixed flat flame

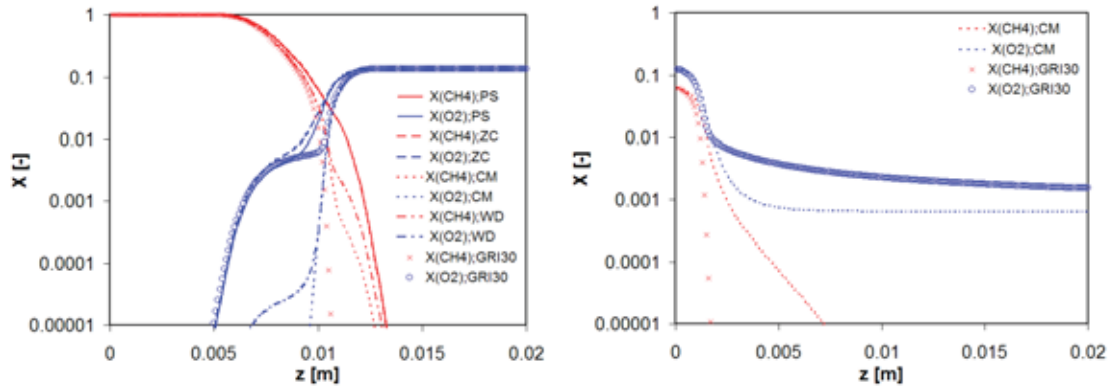

Fig. 6. Predicted volume fraction profiles of reactants in (a) CH_4/Air-Ar nonpremixed counterflow flame and (b) CH_4-Air-Ar premixed flat flame

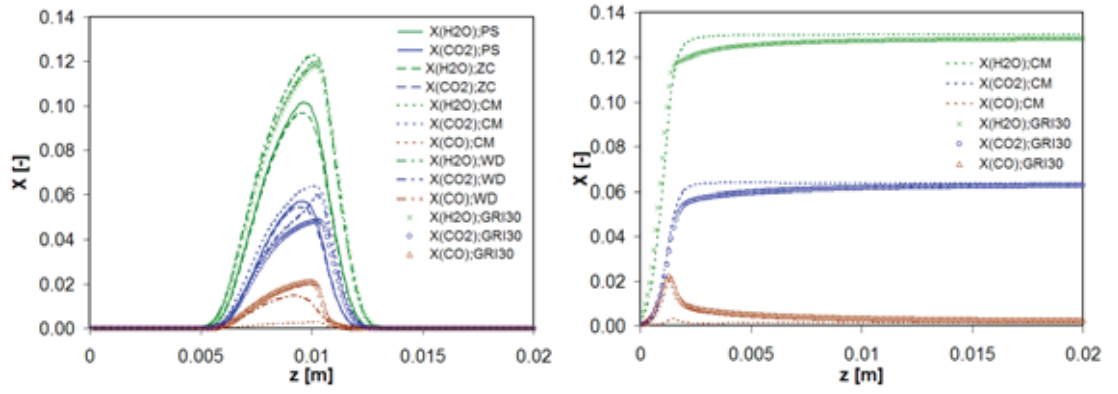

Fig. 7. Predicted volume fraction profiles of product and intermediate in (a) CH_4/Air-Ar nonpremixed counterflow flame; (b) CH_4-Air-Ar premixed flat flame

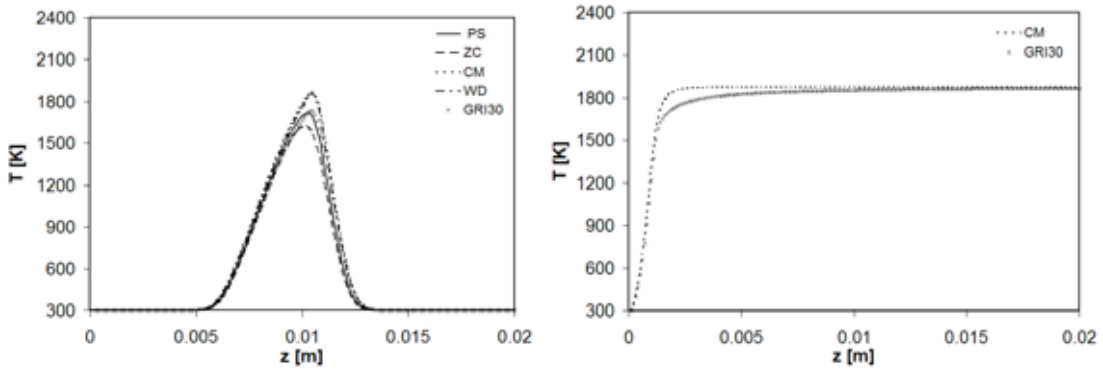

Fig. 8. Predicted profiles of temperatures in (a) CH_4/Air-N_2 nonpremixed counterflow flame; (b) CH_4-Air-N_2 premixed flat flame

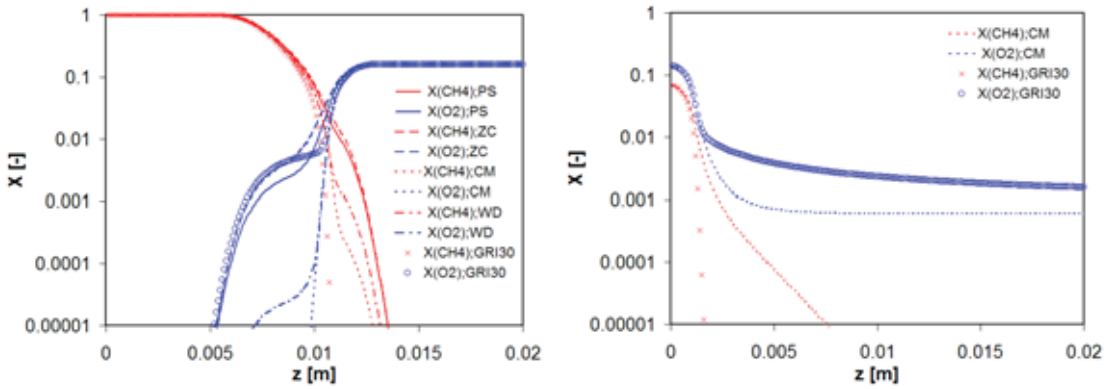

Fig. 9. Predicted volume fraction profiles of reactants in (a) CH_4/Air-N_2 nonpremixed counterflow flame; (b) CH_4-Air-N_2 premixed flat flame

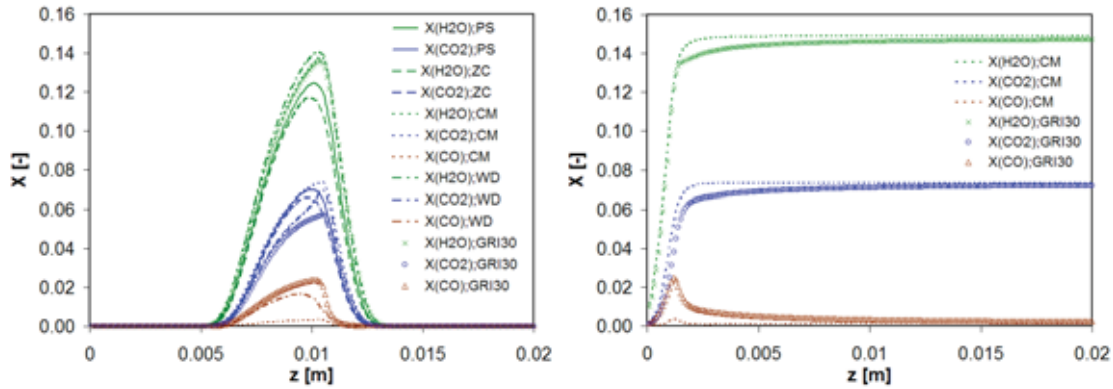

Fig. 10. Predicted volume fraction profiles of products and intermediate in (a) CH_4/Air-N_2 nonpremixed counterflow flame; (b) CH_4-Air-N_2 premixed flat flame

3.4. Laminar flame speed calculations

Laminar flame speed was calculated in Cantera 1.7 environment using freely-propagating premixed flat flame configuration with the same parameters as utilized for burner-stabilized flat flame. The only difference is the boundary condition at $z = 0$ coordinate point enabling the burner exit (mass flow inlet) velocity to get equal to burning velocity sustained by the chemical kinetics (towards the burner) during the iteration process. It should be noted, that the combustion is not sustained, if the flow velocity of fresh gas mixture is dominating over the velocity of flame front propagating in the direction to the burner surface. There are numerous studies considering laminar flame speed as being suitable indicator of the proper performance of chemical kinetic model in premixed combustion condition including the effect of dilution [22,23]. Recent experimental data describing the effect of nitrogen dilution on laminar flame speed of atmospheric-pressure premixed CH_4-air flames are provided by Halter et al. [24]. Perfect agreement of experimental data with laminar flame speeds calculated by freely-propagating flame simulation using GRI-Mech 3.0 [17] was obtained also for the elevated initial temperatures ($T = 393$ K) [25].

Different transport models were employed in laminar flame speed calculations. At high dilution condition the type of transport models is of comparable importance as in the case of undiluted combustion for global models. Decreased sensitivity of laminar flame speed to transport parameters for the detailed chemistry models was identified based on the results shown in Table 7. It is important to note, that even by the simulation of the freely-propagating flame, we was unable to predict the laminar burning velocity for the selected one-step models (PS and ZC). Nevertheless, the CM model performs sufficiently well in premixed flame simulation.

Table 7. The results of laminar flame speed calculations (values are shown in $m.s^{-1}$). The N letter in the table stands for the non-successful iteration process (unavailable data for the given model and conditions)

	Laminar flame speed (mixture-averaged/multicomponent transport)				
Simulation case (Fuel/Oxidizer-Diluent)	PS model	ZC model	WD model	CM model	GRI30 model
CH_4/Air	0.222/0.234	0.166/0.175	0.261/0.272	0.370/0.386	0.347/0.379
CH_4/Air-Ar	N/N	N/N	0.073/0.078	0.136/0.146	0.148/0.153
CH_4/Air-N_2	0.068/0.071	0.068/0.071	0.085/0.088	0.159/0.166	0.160/0.163

3.5. Simulation of moderately diluted nonpremixed (CH_4/Air-Ar) flame

Two-dimensional computational domain consisting of 10 000 rectangular cells with uniform grid size of 0.2 millimetres was used for the CFD simulation case study. Moderately diluted CH_4/Air-Ar nonpremixed counterflow flame, with $X(\mathrm{Ar}) = 0.186$ at oxidizer inlet, was considered to be the representative case for the testing purposes. This volume fraction of diluent (argon) corresponds the one half of the minimum extinguishing concentration, $X(\mathrm{Ar})_{ext}$. Laminar flow model together with finite-rate chemistry assumption applied in ANSYS Fluent 14.0 excluding the effects of turbulence and influence of turbulence-chemistry interactions. The combination of stiff chemistry solver with the SIMPLE iteration scheme was utilized in order to facilitate the process of convergence.

One-step PS model was selected to provide initial estimate for describing the reaction zone at this level of dilution. The default values of thermodynamic parameters (in the form of 5-th order polynomials) as well as the transport data from the database of ANSYS Fluent 14.0 were used for this simulation. One-dimensional simulations were performed with analogous boundary conditions. The temperature profile

was also predicted using detailed chemistry model (GRI30) in Cantera 1.7. The results of these simulations together with the data obtained by CFD simulation are plotted in Fig. 10.(b). If we compare the detailed kinetic model (GRI30) data with prediction of PS model using Cantera 1.7, the results are qualitatively to undiluted flame simulations discussed above and presented in Fig. 2.(a). Therefore, for moderate argon dilution, the one-step PS model is able to predict reliably the position (mainly the fuel-lean side) of reaction zone in contrast to its performance in highly diluted flames. Temperature overprediction is significant in moderate argon dilution case, but lower than for the flame without dilution, see Fig. 10.(b). To keep the consistency with above presented plots, the temperature profile is shown in z-axis coordinate, which is in fact x-axis for two-dimensional simulation in ANSYS Fluent 14.0. Centreline (horizontal line $y = 0.01$ m) temperature profile is used here for the comparison.

Systematic shift of reaction zone towards the fuel-rich side can be observed in the results of CFD simulations (using PS model in ANSYS Fluent 14.0). Several factors can contribute to different prediction of temperature on fuel-lean side of reaction zone, including the formulation of balance equation, thermodynamic and transport properties.

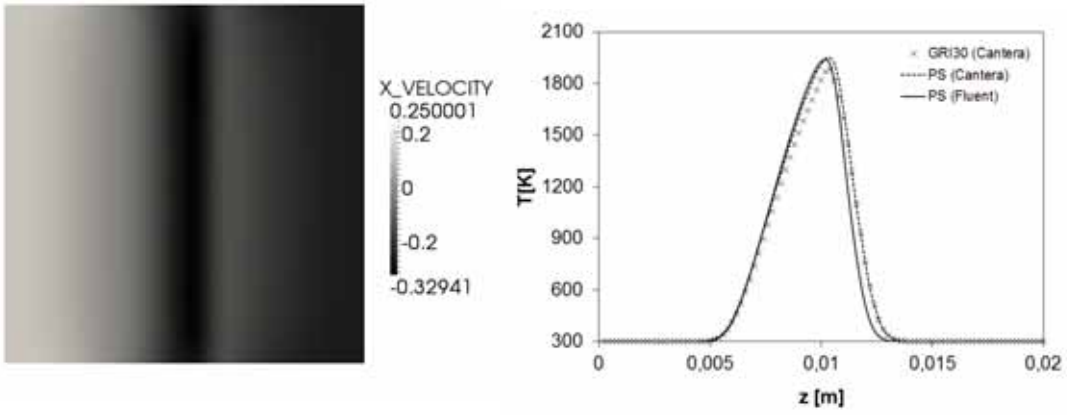

Fig. 11. The plots of quantities obtained for moderately diluted CH_4/Air-Ar nonpremixed counterflow flame (a) axial velocity component in computational domain predicted by ANSYS Fluent 14.0 using one-step PS model; (b) the centreline temperature profiles obtained by using one-step PS model in ANSYS Fluent 14.0 and the results of predictions using PS and GRI30 model in Cantera 1.7.

The magnitude of varying thermodynamic or transport parameters and their formulations needs to be investigated in details. This study is currently in progress (will be reported elsewhere). The comparison of computational tools involving the methods of sensitivity analysis is further required to explain the discrepancies of model predictions.

4. Conclusion

The effect of elevated concentration argon and nitrogen in flame involves mainly the heat extraction and dilution phenomena. Reduction of temperature in the reaction zone of highly diluted laminar premixed and nonpremixed flames was quantitatively estimated based on mathematical modelling. The reliability of global chemistry models is changing considerably as dilution effect increase. For nonpremixed flames one-step models can provide satisfactory estimate of maximum temperature in the reaction zone for moderate dilution of oxidized stream. At least, two-step chemical kinetics models should be preferred for predicting the temperature and concentration of major species in premixed flames

adequately. The ability to predict the laminar flame speed properly even in the highly diluted conditions is the qualitative measure of the model performance in premixed combustion.

Beside the practical aspects of this study, investigations of the chemical kinetics and fluid flow physics under reduced temperature conditions provide important information for model development and validation strategies. Availability of reliable modelling tools and data suitable for predicting the structure of reaction zone in such conditions is crucial for understanding the phenomena involved in transient (oscillating or turbulent) chemically reacting flows.

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